

## **Toward Predictive NanoMaterial Design**

### **(Experimentation, Metrology, EHS, Modeling and Critical Algorithms)**

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**Background:** One of the most fundamental needs for nano-manufacturing to become viable is to understand and control the factors in nano-material synthesis that determine nanoscopic through macroscopic materials properties. The chemical and semiconductor industries have identified joint nanotechnology research needs which would enable the correlation and prediction of nanostructure and properties from synthetic conditions. Industrial sectors such as Aerospace and Automotive have also articulated similar needs. However, the development of such predictive models will require a great deal of experimentation, development of new metrology methodologies, instrumentation and the creation and enhancement of new algorithms. Models are needed that provide a framework for the systematic characterization of synthetic methods and material properties, which are sufficient to enable the retro-synthetic design of useful materials with a multiplicity of desired properties while keeping in mind the environmental, health and safety aspects of the manufacturing processes employed..

Many nanomaterial modeling and characterization efforts are under way at universities and national laboratories internationally. Unfortunately, these initiatives currently lack the coordination and levels of support that are required to develop these capabilities into an integrated resource with broad utility. No one agency or institution has the scope or resources to satisfy these predictive materials by design need. Many industries, including aerospace, energy, automotive, chemical, electronics, etc., would value the development of such a predictive modeling capability and nanotechnology design infrastructure that delivers high performance materials with superior properties. Additionally, this modeling infrastructure also would support and enhance the government's ability to achieve mission critical goals.

This meeting's goals are to identify:

1. Collaborative pathways and resources within and among different research institutions, which are currently developing and characterizing these models;
2. Perceived coordination and resource gaps that are barriers to achieving an interdependent and sufficient predictive modeling infrastructure;
3. Prioritize collaborative opportunities for multiple institutions and agencies to develop this materials modeling by design capability. Specifically, what

is the best way to utilize the strengths of different research institutions to develop these enabling capabilities?